

UNITED STATES PATENT APPLICATION

of

ARTHUR J. PITERA

and

EUGENE A. FITZGERALD

for

**COPLANAR INTEGRATION OF LATTICE-MISMATCHED
SEMICONDUCTOR WITH SILICON VIA WAFER BONDING VIRTUAL
SUBSTRATES**

**COPLANAR INTEGRATION OF LATTICE-MISMATCHED
SEMICONDUCTOR WITH SILICON VIA WAFER BONDING VIRTUAL
SUBSTRATES**

5

PRIORITY INFORMATION

This application claims priority from provisional application Ser. No. 60/391,555
June 25, 2002, which is incorporated herein by reference in its entirety.

BACKGROUND OF THE INVENTION

10

The invention relates to the field of virtual substrates, and in particular to coplanar
integration of lattice-mismatched semiconductors with silicon via wafer bonding virtual
substrates.

15

The large lattice constant mismatch between Si and GaAs/Ge precludes direct
growth of the mismatched material directly on Si without nucleation of a high density of
defects. One solution to this limitation is growth of compositionally graded layers where
a large lattice constant mismatch is spread across several low-mismatch interfaces,
thereby minimizing nucleation of threading dislocations. Compositional grading of
relaxed $\text{Si}_{1-x}\text{Ge}_x$ layers of increasing Ge fraction can be used to create an arbitrary lattice
constant ranging from that of Si to Ge on a bulk Si substrate. Such a structure is termed a
virtual substrate.

20

25

Ge virtual substrates could further be used to integrate GaAs with Si since the
lattice mismatch between Ge and GaAs is low. Unfortunately, the virtual substrate
approach has the disadvantage of requiring a thick graded buffer to ensure complete
relaxation of the individual mismatched layers. In the case of Ge virtual substrates,
which are graded from Si to pure Ge, the buffer thickness is typically greater than $10\mu\text{m}$.

Such thick layers 2 result in severe wafer bow due to thermal stress and complicate integration of the mismatched material with the underlying Si 4 since the device levels are not coplanar and must be interconnected across a deep step, as shown in FIG. 1.

Wafer bonding and layer transfer is another approach for integrating low-defect, lattice mismatched materials, as shown in FIG. 2. In this approach, two flat, clean wafer 6, 8 surfaces are brought into contact and annealed at high temperatures to create a strong bond. A thin layer of material is then transferred from the seed wafer to the handle wafer by means of grind and etch-back with the aid of an etch-stop layer or layer exfoliation by hydrogen ion implantation. However, the differing coefficients of thermal expansion (CTE) of Si relative to GaAs and Ge limit the annealing temperature that these bonded pairs can be exposed to. In addition, wafer size mismatch limits their use to non-leading edge fabrication facilities.

SUMMARY OF THE INVENTION

According to one aspect of the invention, there is provided a method of bonding lattice-mismatched semiconductors. The method includes forming a Ge-based virtual substrate and depositing on the virtual substrate a CMP layer which is polished to form a planarized virtual substrate. Also, the method includes bonding a Si substrate to the planarized virtual substrate and performing layer exfoliation on selective layers of the planarized virtual substrate producing a damaged layer of Ge. Furthermore, the method includes removing the damaged layer of Ge.

According another aspect of the invention, there is provided a method of bonding lattice-mismatched semiconductors. The method includes forming a Ge-based virtual

substrate. Also, the method includes using the virtual substrate to form a planarized virtual substrate and bonding a Si substrate to the planarized virtual substrate. Furthermore, the method includes removing selective layers of the planarized virtual substrate associated with the Ge-based virtual substrate.

5

BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1 is a schematic block diagram demonstrating the issue of non-coplanarity arising when SiGe virtual substrates are used to integrate Ge or GaAs with Si;

FIG. 2 is a schematic block diagram demonstrating wafer diameter mismatch
10 between Si and Ge/GaAs;

FIG. 3 is a schematic block diagram demonstrating growth of flat virtual substrates via film stress engineering;

FIG. 4 is a schematic block diagram demonstrating thermal stress balancing by virtual substrates growth using double-polished wafers;

15 FIG. 5 is an AFM micrograph of an as-grown Ge virtual substrate;

FIG. 6 is a graph demonstrating material removal rate vs. Ge fraction in $\text{Si}_{1-x}\text{Ge}_x$ films using a standard Si CMP process;

FIG. 7 is an AFM micrograph of a Ge virtual substrate polished using a standard Si CMP process;

20 FIG. 8 is a cross-sectional TEM micrograph of an epitaxial Si CMP layer grown on a Ge virtual substrate;

FIGs. 9A-9F are schematic block diagrams demonstrating the Ge film transferring process;

FIG. 10 is a cross-sectional TEM micrograph of the GOI structure after layer transfer and selective etching;

FIGs. 11A-11B are AFM micrographs demonstrating the surface morphology of the transferred Ge film before and after selective etching; and

5 FIG. 12 is a cross-sectional TEM micrograph showing Ge on Si transferred from a Ge virtual substrate.

DETAILED DESCRIPTION OF THE INVENTION

The invention provides a technique to obtain coplanar integration of high-quality,
10 lattice-mismatched materials on large diameter substrates using a combination of virtual substrate growth and wafer bonding via a planarization layer and layer exfoliation by H_2^+ ion implantation. By using a virtual substrate as the seed wafer, the bond annealing temperature is not limited by the CTE mismatch of the bonded pair since bulk composition of both wafers in the bonded pair is the same. Furthermore, since the graded
15 buffer is grown on Si, mismatched layers can be transferred to large diameter Si wafers.

Prior to wafer bonding Ge virtual substrates, several issues including wafer bow, surface roughness, low thermal budget and layer transfer must be resolved. These issues will be addressed in the following sections.

Prior to wafer bonding, the virtual substrates must be engineered to be flat. The
20 CTE mismatch between Si and SiGe alloys creates wafer bow, which can exceed $40\mu m$ deflection in Ge virtual substrates fabricated with a 100mm wafer. Although the higher CTE of Ge compared to Si results in SiGe films that are under tensile thermal strain, the larger lattice constant of SiGe can be used to grow metastable films that are

compressively lattice strained. A compressively strained Ge cap 14 can be created by increasing the final composition step in the graded buffer 12 while decreasing the growth temperature to suppress dislocation glide kinetics, as shown in FIG. 3. The stress in the tensile graded buffer 12 and compressive Ge cap 14 can therefore be engineered to yield
5 a flat substrate 10.

A second solution to wafer bow is used to grow the SiGe buffers 18, 20 on both sides of a double-side polished substrate 16, as shown in FIG. 4. This solution could be applied to hot-walled growth systems as film deposition must occur on both sides of the wafer. In this case, the tensile strain of the SiGe layers 18 on one side of the wafer
10 exactly offsets that of the other 20 yielding a flat substrate 22.

As-grown Ge virtual substrates exhibit a crosshatch pattern characteristic to graded buffer growth. The crosshatch pattern 24 of a typical Ge virtual substrate is shown in FIG. 5.

These substrates typically have a roughness of 10-15nm RMS as measured on a
15 10×10μm scale. This roughness must be reduced to less than 0.5nm for efficient mating of the bonding surfaces. The $\text{Si}_{1-x}\text{Ge}_x$ virtual substrates with a Ge fraction of up to 60% can be readily planarized using a standard Si chemo-mechanical polishing (CMP) process consisting of a KOH-stabilized colloidal silica. However as the virtual substrate composition is increased to pure Ge, the material removal rate (MRR) decreases to less
20 than 0.5Å/sec making planarization of Ge highly inefficient. The decrease in polish rate with increasing Ge fraction is shown in FIG. 6.

The combination of low polish rate and anisotropic etching causes pitting due to preferential removal of material around dislocations threading to the surface. These

surface pits 26 along with incomplete removal of the surface roughness can be seen in a 25×25μm AFM scan, as shown in FIG. 7.

Furthermore, bulk Ge polishing techniques cannot be applied to Ge virtual substrates since these methods rely on chemical polishing and require removal of a large amount of material to achieve the required surface roughness. The cap thickness of Ge virtual substrates typically cannot exceed 2μm due to thermal stress limitations.

In this process, CMP of the Ge virtual substrate is facilitated with a planarization layer consisting of an epitaxial Si_{1-x}Ge_x layer or deposited oxide. This layer not only aids surface planarization, but also serves to protect the Ge surface from subsequent post-CMP and pre-bonding cleaning steps.

An epitaxial Si layer with a nominal thickness of 2μm is used to planarize the virtual substrate 30, as shown in FIG. 8. The 4% lattice mismatch between Si and Ge causes nucleation of a high density of dislocations in the planarization layer 28. However, these defects stay confined to the Si and do not enter the underlying Ge 32 as illustrated in the cross-sectional TEM micrograph shown in FIG. 8. It is important to realize that the Si serves only as a planarization layer and its defect content is inconsequential to the device layers, which will be fabricated on the transferred Ge. However, SiO₂ can also be used in planarizing a virtual substrate.

Activation of strong hydrophilic Si to Si bonding occurs at annealing temperatures exceeding 800°C. These temperatures approach the melting point of Ge, therefore it would be beneficial to reduce the annealing temperature of bonded Ge virtual substrates without sacrificing bond strength. Use of plasma-activated wafer bonding can

be made to achieve high strength wafer bonds with annealing temperatures lower than 400°C.

After bonding the planarized seed wafer to the Si handle, the virtual substrate must be removed to transfer the Ge layer. In general, this can be done by mechanical
5 thinning of the seed wafer to a final thickness of approximately 50µm. The remaining material is then chemically etched away with the aid of a built in etch stop layer which terminates material removal at the desired thickness. A KOH or TMAH etch can be used to preferentially etch $\text{Si}_{1-x}\text{Ge}_x$ to a Ge fraction of about 20%. However, for Ge virtual
substrates, a method for removing the remainder of the buffer must be devised as shown
10 in FIGs. 9A-9F.

FIGs. 9A-9F show the Ge film transfer process incorporating an etch-stop and an oxide CMP layer 44 for use as a planarization layer. In other embodiments, the CMP layer 44 can be Si, as discussed herein. After UHVCVD growth of the virtual substrate and Ge transfer structure 38 that also includes a passivation layer composing of a material
15 such as Si_3N_4 or $\text{Si}_{1-x}\text{Ge}_x$ with a nominal value of $x=0$ 44, an SiO_2 layer with a nominal thickness of 7500 34 is deposited at 400°C using low pressure CVD (LPCVD) and densified at 650°C, as shown in FIG. 9A. The wafer 40 is then CMPed reducing the oxide thickness to a nominal value of 2500Å and implanted with H_2^+ to a dose ranging between $1 \times 10^{16} \text{cm}^{-2}$ and $1 \times 10^{17} \text{cm}^{-2}$ with a nominal dose of $4 \times 10^{16} \text{cm}^{-2}$ shown in FIG.
20 9B. The implant energy should be sufficient to penetrate layers 34, 44, 46, 36 and 50. Prior to bonding the virtual substrate 38 to a Si handle wafer 42, both substrates 38, 42 are given a chemical cleaning treatment such as 3 H_2SO_4 : 1 H_2O_2 for 10 minutes followed by a DI water rinse and spin dry, leaving both surfaces hydrophilic, as shown in

FIG. 9C. At this point, the wafers 40, 42 may be given a plasma treatment, typically in an O₂ plasma, as an additional surface activation step to improve the bond strength obtained during annealing temperatures below 800°C. Next, the wafers 40, 42 are direct bonded and annealed at a nominal temperature of 250°C for a nominal time of 12 hours to strengthen the bond. Layer exfoliation is carried out at a temperature ranging between 300 and 650°C with a nominal temperature of 450°C, transferring the CMP layer 34 Ge 46, 50, passivation layer 44 and etch-stop 36 layers to the Si handle wafer 42, as shown in FIG. 9D. Finally, the transferred film structure 52 is etched in H₂O₂ to selectively remove the damaged Ge surface 50, as shown in FIG. 4E. A selective CMP step could be applied to remove the remaining etch stop layer 36, as shown in FIG. 9F.

The Si_{0.4}Ge_{0.6} etch-stop layer 36 places an upper limit on the thermal budget for our film-transfer process. Annealing experiments reveal that the buried Si_{0.4}Ge_{0.6} layer 36 is lost to interdiffusion after a 650°C anneal for >6 hours, after which it no longer exhibits etch-stopping behavior. It was therefore necessary to tailor our layer transfer process to stay within the bounds of this thermal budget.

FIG. 10 shows a cross-sectional TEM micrograph of a GOI structure after layer transfer and selective etching. This is the first demonstration of high-quality epitaxial Ge transfer from a virtual substrate to Si. Using the buried etch-stop layer 64, the surface damage induced by the Ge exfoliation process is removed using a selective etch rather than a CMP process, allowing for very precise control of the transferred Ge thickness 66. The thickness 66 of the transferred Ge layer 68 is defined by the etch-stop layer 64, which is located at the surface of the structure 70 in FIG. 10. The thickness 66 of the transferred Ge layer 68 is 1400Å. The reverse selectivity of our CMP process can be

used to remove the Si-rich etch-stop relative to the underlying Ge device layer, leaving a damage-free Ge surface for device fabrication.

As described herein, the virtual substrates are capped with a thin Si passivation layer 70 to protect the Ge surface during wafer processing. Because this layer 70 is epitaxially grown directly on Ge, it contains a high density of defects resulting from the 4% mismatch between Si and Ge. After bonding and film transfer, this layer 70 becomes buried between the LTO and Ge layers in the final structure as seen in FIG. 11. The effect of the passivation layer 70 will be device-specific and no conclusions can be made until actual devices are fabricated. However, it is speculated that since the passivation layer 70 is very thin ($<100\text{\AA}$) compared to the Ge device layer 68, the defects confined to the Si will only have a small, if any effect on devices fabricated on this material. Furthermore, the Si/SiO₂ interface 72 is electrically superior to that of Ge/SiO₂, therefore the presence of the passivation layer 70 may be beneficial in this respect. In any case, for the purpose of surface passivation 70 an alternate material such as a layer of deposited Si₃N₄ instead of epitaxial Si could be used for future GOI fabrication schemes if required for devices fabricated on these substrates.

The surface morphology of the transferred film before and after selective etching is shown in FIGs. 11A-11B. FIG. 11A shows the exfoliation damage of the as-transferred Ge film. At this stage the surface of the transferred Ge layer is heavily damaged and exhibits a surface roughness $>50\text{nm RMS}$, measured over a $25\times 25\mu\text{m}$ area.

After selective peroxide etching, the surface roughness is reduced to $<15\text{nm RMS}$ and the crosshatch pattern of the original virtual substrate is revealed as shown in FIG. 11B. It is interesting to note that the re-emergence of the crosshatch is not caused by

anisotropic etching but is a result of the $\text{Si}_{0.4}\text{Ge}_{0.6}$ etch-stop layer being grown on a crosshatched surface prior to planarization. When the peroxide etch reaches the etch-stop layer, an inverted version of the original crosshatch pattern is delineated in the transferred film. Comparing the surface morphology of the original virtual substrate with the
5 transferred and etched Ge layer, the surface roughness is reduced from 30 to 1.4nm RMS as determined from a $1 \times 1 \mu\text{m}$ AFM scan.

The high surface roughness of the as-transferred film is attributed to the large stopping distance associated with the 200keV energy used to implant H_2^+ for layer transfer. This exfoliation-induced roughness is completely removed after selective
10 etching; however lower implant energies could be used to minimize the surface damage. This is particularly achievable if the thickness of the oxide CMP layer is reduced or removed entirely. The latter requires direct CMP of the Ge virtual substrate, which if done prior to growth of the etch-stop and Ge transfer layers, will result in a crosshatch-free surface morphology in the transferred Ge film. However, this optimal solution will
15 not be possible until planarization techniques for Ge virtual substrates are perfected.

The invention uses a specific process for integrating Ge layers directly on large diameter Si wafers. However, a number of variants to this approach can be envisioned which could yield an assortment of engineered substrates. The structure fabricated in this invention could be used as-is for integration of Ge photodetectors or subsequent growth
20 of GaAs for III-V integration. The combination of layer exfoliation and Ge-selective etching could also be useful for ultra-thin strained SiGe/Ge layers integrated directly on insulator. Strained SiGe/Ge layers have been shown to have greatly improved hole mobility over conventional Si. Further benefits could be gained by fabricating such

layers on insulator. Since this process does not require CMP of the device layer, the thickness of the transferred film is defined entirely by epitaxy thus allowing for fabrication of ultra-thin layers directly on insulator.

In a different embodiment, FIG. 12 shows a 1 μ m thick Ge layer, which is transferred to Si from a Ge virtual substrate with the aid of an epitaxial Si planarization layer, but without the use of a buried etch-stop layer. The virtual substrate is created using hot-walled UHVCVD deposition of compositionally graded Si_{1-x}Ge_x layers on a double-polished Si wafer, resulting in wafer deflection <15 μ m across a 100mm wafer. The Si planarization layer is allowed application of a standard Si CMP process to planarize the surface prior to wafer bonding.

To minimize thermal budget, both seed and handle wafers are exposed to O₂ plasma for 1min and rinsed in DI water for 5 min after receiving a modified RCA clean consisting of 10 min (3H₂SO₄:1H₂O₂) and 15 min (6H₂O:1HCl:1H₂O₂), 80°C. Layer transfer is carried out by implanting the wafers with H₂⁺ ions at an energy of 200keV and a dose of 4 \times 10¹⁶cm⁻² prior to wafer bonding. After an initial 12 hour anneal at 250°C, the Ge layer was exfoliated by annealing at a temperature of 500°C for 10min. The layer exfoliation process left a 7000Å damage layer 60, which could be removed by chemical etching incorporating a Si_{1-x}Ge_x etch stop layer in the cap of the Ge virtual substrate.

III-V compounds could be similarly integrated directly on a Si substrate by growing GaAs on a Ge virtual substrate and transferring it to Si by wafer bonding and layer exfoliation. The GaAs device layer could then be used as an etch-stop to selectively remove the Ge with a hydrogen peroxide etch. Extending this process to III-V compounds, it is possible to compositionally grade in the In_xGa_{1-x}As system for

integration of semiconductor materials with lattice constants larger than Ge. These include materials such as InP and InAs, which have useful electronics and optoelectronic applications. Ultimately, wafer bonding virtual substrates will offer the flexibility of integrating virtually any material directly on large diameter Si wafers, thus eliminating
5 the limitations of Si and dramatically increasing the functionality of CMOS for high performance electronics and optoelectronics applications.

Although the present invention has been shown and described with respect to several preferred embodiments thereof, various changes, omissions and additions to the form and detail thereof, may be made therein, without departing from the spirit and scope
10 of the invention.

What is claimed is: